A Multimaterial Numerical Method for Eulerian Shock Physics

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The hydrodynamic techniques used for shock physics analysis in Sandia National Laboratories hydrocodes are based upon fundamental staggered mesh artificial viscosity methods originating in the 1950's and 1960's. While this technology has stood the test of time, advanced numerical algorithms for compressible fluid dynamics have been developed in recent years. Most of these methods employ solution algorithms that do not extend easily to multidimensional, multimaterial and/or nonideal equations of state. A description of the fundamental conservation equations describing multimaterial hydrodynamics is presented. The equation set contains additional constraints and conservation equations that require special numerical algorithms to address the implicit embedded time and length scales. This formulation provides a physics and mathematics based approach for simulating the complex shock wave propagation through regions of space occupied by multiple materials. Progress toward implementing the additional conservation equations and constraints is presented and sample numerical simulations are illustrated.

Introduction

The increase in computational power in recent years has made analysis of complex multidimensional shock wave propagation problems common place. In addition, new experimental methods and theoretical investigations are shedding light on the nature of the complex wave phenomena (Baer, 2003). Mathematical descriptions are being developed to simulate the complex behavior at multiple length and time scales (Baer and Nunziato, 1986). The new mathematical models are pushing the limits of the currently available computational technology. Research into numerical methods has resulted in a collection of new and innovative techniques (Andrianov, 2003, Baty, 1994, Crawford, 2005, Miller and Colella, 2001, Miller and Colella 2002, Miller and Puckett, 1996, Saurel and Abgrall, 1999, Stone and Norman, 1992, Yee, 1987). Pure Eulerian methods are appealing due to the multitude of research that forms the foundation of these procedures (Van Leer, 1977, Oran and Boris, 1987). However, the majority of the new methods are not applicable to multidimensional, multimaterial shock propagation through complex nonideal materials. As the new technology matures it is necessary to investigate the foundations of the current methods and extend these techniques to meet near term goals.

A proven strategy for simulating the large deformation wave propagation with multiple complex materials is to use a Lagrangian physics step followed by an Eulerian

remap method (Crawford, 2005). This technology has been demonstrated through numerous experimental comparisons to capture the salient features associated with shock physics problems. There is an open debate regarding the detailed validation of the numerical methods and the corresponding verification of the various physics model implementations. It is often not the scientific technical details that are in question, but the resulting art of implementation and algorithmic approximation that is questioned. Most hydrocodes are equipped with a set of control parameters that allow fine tuning of the computation for certain classes of problems. Ultimately a skilled user of the computational tool will be able to obtain reasonable results by manipulating these controls. However, it is often the case that detailed investigation unravels the underlying ad hoc processes that lead to development and implementation of the controls.

One specific aspect of multimaterial Eulerian shock physics codes that needs to be addressed is the treatment of mixed cells. A mixed computational cell is defined as a single cell that contains two or more materials. For practical problems it is often the assumptions and approximations that are made for this class of computational cell that result in numerical issues. The numerical issues are then addressed using further ad hoc algorithms or even discard options to eliminate "bad" material. There are a series of approximations that can be employed to represent the response of mixed material cells. For example, it can be assumed that all materials in a cell have the same pressure and temperature, the same pressure and different temperature, or different pressures and temperatures. Each level of approximation can be used to obtain useful results for a given application. However, it is easy to demonstrate that each option may lead to erroneous results if it is not carefully applied. In the authors opinion the approximations that are made to the governing conservation equations suffer from an arbitrary nature, but are currently necessary to allow efficient solution to this problem class.

A traditional approach to multimaterial hydrodynamics is presented (Fromm, 1961, McGlaun, 1987). Current methods to provide mathematical closure to the governing equations are illustrated. A new set of governing equations and a numerical solution procedure is presented. This procedure requires efficient stiff solvers to resolve the complex phenomena associated with subgrid-scale processes (Mott and Oran, 2001, Shampine and Watts, 1980). An example of this subgrid scale process is the temperature relaxation between mixed materials in a cell. The heat transfer can be characterized by time scales that are significantly different than the Courant limited hydrodynamics time step.

Governing Equations

The multimaterial representation of the Euler equations written in conservation form is:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0 \qquad [1]$$

$$\frac{\partial (\rho V)}{\partial t} + \nabla \cdot (\rho V \otimes V + P) = 0 \qquad [2]$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho E V + P V) = 0 \qquad [3]$$

The mixture density ρ is defined as

$$\rho = \sum_i \phi_i \gamma_i \qquad [4]$$

The volume fraction is ϕ and the true density is γ. The cell pressure is defined as,

$$P = \sum_i \phi_i P_i \qquad [5]$$

The total energy is defined as

$$\rho E = \sum_i \phi_i \lambda_i \left(e_i + \frac{1}{2} V \cdot V \right) \qquad [6]$$

The specific internal energy, e_i, is determined by partitioning the total energy into each material. This equation set is augmented with an equation of state of the form pressure is a function of the true density and specific internal energy.

- This set of equations with the following unknowns (P, ϕ, γ, e, V) is closed mathematically by making an assumption regarding the evolution of the volume fraction. The most common assumptions made are that the pressure and temperature of all of the materials in a computational cell have the same value, or the pressure of all materials is the same with a different value of the temperature, or the pressure and temperature of all materials are different. When the pressure and /or the temperature are fixed between materials in a computational cell the volume fraction is forced to adjust to this assumption. That is, the density and the energy of each material are modified such that the pressure and/or temperature of all materials are the same. This adjustment does not follow any physical laws and represents an ad hoc assumption regarding the physical nature of materials in a computational cell. If the pressure and temperature are assumed to evolve independently then algebraic rules are used to approximate the energy/volume partitioning within multimaterial cells. The algebraic rules may be derived from compressibility arguments or other simplistic mixture approximations, but are still ad hoc.

- A common assumption used in continuum mixture theory is that the volume fraction has an evolutionary equation in the form of an advection equation with a source term (Truesdell, C., 1984). The form of this equation as outlined in Baer and Nunziato (1986) is,

$$\frac{\partial \phi_s}{\partial t} + V_s \cdot \nabla \phi = \frac{f(\phi)}{\mu} \left[P_s - \beta_s - P_g \right] \qquad [7]$$

where the subscript "s" implies a solid phase and "g" implies a gaseous phase, β_s represents a configurational stress, and μ is a compaction viscosity. This equation states

that along a solid-phase streamline the solid volume fraction relaxes viscously toward an equilibrium state defined by the configurational stress and the gas-phase pressure. The advantage of a multiphase formulation is that each phase has a set of conservation equations with a source term representing interphase exchange of mass, momentum, and energy. Each phase also has its own velocity field. The critical aspect in the application of continuum mixture theory is the determination of the interphase source terms consistent with the second law of thermodynamics. There are other mathematical formulations of multimaterial hydrodynamics that encompass a volume fraction evolution equation (Miller and Puckett, 1996). The various equations differ in the methods used to specify the source term. The particular form used in this paper is,

$$\frac{\partial \phi_i}{\partial t} + V \cdot \nabla \phi_i = \frac{f(\phi)}{\mu} \left[P_i - \beta_i - P_j - \beta_j \right] \qquad [8]$$

The Lagrangian evolution of the volume fraction of material "i" viscously relaxes toward the equilibrium state in the cell. The assumption made here is that there is one velocity for all materials in a computational cell. This approximation will be assessed in future work. Equations 2, 3, 6, and 8 can be combined to derive an equation for the change in the specific internal energy of material "i." The "j" index represents another material in the cell.

$$\phi_i \gamma_i \frac{\partial e_i}{\partial t} + \phi_i \gamma_i V \cdot \nabla e_i = \phi_i P_i \nabla \cdot V + \left[P_i - \beta_i - P_j - \beta_j \right] \phi_i' + H(T_i - T_j) \qquad [9]$$

The first term on the righthand side of Eq. [9] represents the material work due to hydrodynamic motion, the second term is an intermaterial work term and the last term represents intermaterial heat transfer. The goal is to develop numerical techniques to solve Eqs. (1-3, 8-9). Models for representing the configurational stresses are under development and will be the subject of future work. The motivation for development of the volume fraction evolution equations is to represent the physics of various nonequilibrium processes with more fidelity. Some of the processes under consideration are pressure relaxation, heat transfer, chemical transformation, phase transformation, porosity evolution, configurational effects, and fracture mechanics. The nature of the various processes under consideration here is represented by time-dependent kinetic relaxation toward a state of equilibrium. The implication of these processes is that they represent a continuum of time scales with associated mathematical stiffness.

Numerical Method

➢ A demonstrated strategy for numerical resolution of this highly coupled equation set is to apply time splitting (Oran and Boris, 1987) which is also known as the method of fractional steps (Yanenko, 1971). Three operators are defined to split the time integration between the hydrodynamic step and the source term step. The hydrodynamic step is itself operator split between a Lagrangian physics step and an Eulerian remap step. The Lagrangian and remap steps solve the governing equations without source terms using a standard numerical method such as presented in McGlaun (1987). The operator for time integration of the volume fraction evolution equations with the source terms is

represented by numerical integration of a set of coupled ordinary differential equations. It is necessary to investigate the order of application of these three operators to determine the proper sequence for accurate results. Three sequences of operators that are easily investigated for this approach are,

$$\begin{aligned} &L_\phi L_L L_\phi L_R \\ &L_\phi L_L L_R \\ &L_L L_\phi L_R \end{aligned} \qquad [10]$$

where the Lagrangian hydrodynamic operator is L_L and the Eulerian remap operator is L_R and the volume fraction operator is L_ϕ. Additional sequences of operators may be possible to more closely represent the underlying mathematical structure of the governing equations.

Results

➢ Normal one-dimensional shock propagation problems have a limited number of multimaterial cells that require the volume fraction evolution process. For these problems a minor difference in the time evolution of the material pressure near multimaterial interfaces is observed. This difference is considered insignificant compared with the underlying numerical approximations that are made to create and resolve shock waves. Two of these numerical approximations are associated with the use of nonlinear flux limiting and the use of artificial viscosity. It is difficult to create simple one-dimensional problems with underlying numerical issues associated with the volume fraction assumptions. One particular more complex problem that illustrates incorrect numerical results is the flyer plate impact of a saturated two-material region as illustrated in Figure 1. The two-material region is composed of 10% by volume high impedance material (copper) and 90% low impedance material (air). The numerical results presented in Figure 2 illustrate an unstable wave propagating with an approximate wave speed of 3.75 mm/μs. The solid (black) line represents the mixture average pressure and the dashed (blue) line represents the low impedance material and the remaining lightly shaded (red) line represents the high impedance material. This wave speed corresponds to the higher impedance material behaving as if it is in a separated flow configuration. The two materials in the multimaterial region have different pressures and temperatures throughout the impact problem.

➢ Incorporating the integration of the volume fraction evolution equation stabilizes the wave propagation as illustrated in Figure 3. The wave speed is reduced to approximately 0.75 mm/μs. This result is consistent with mixture averaged wave speed estimates using continuum mixture theory. The viscous relaxation between the components in the two material regions creates a dispersive wave that mimics a mixture equilibration process. Investigation of the order of application of the operator splitting suggests that the first and third forms presented in Eq. 10 are superior to the middle form. The middle form suffers from the fact that only the initial data are available for integrating the volume fraction equations. The completion of the operators for the hydrodynamic cycle introduces significant changes in the density and energy states of the

materials in mixed cells associated with information that is not available at the beginning of the time step.

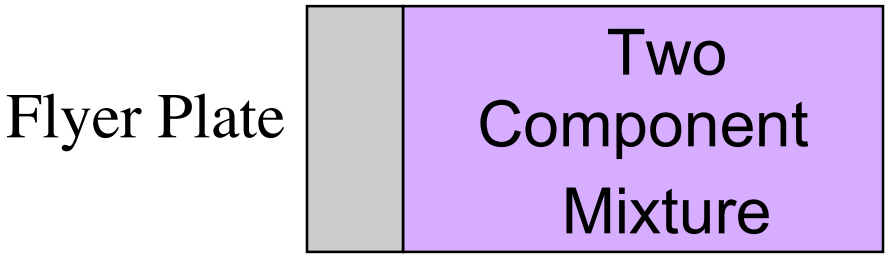

Figure 1. Initial conditions are shown for the flyer plate impact into a saturated two-material region.

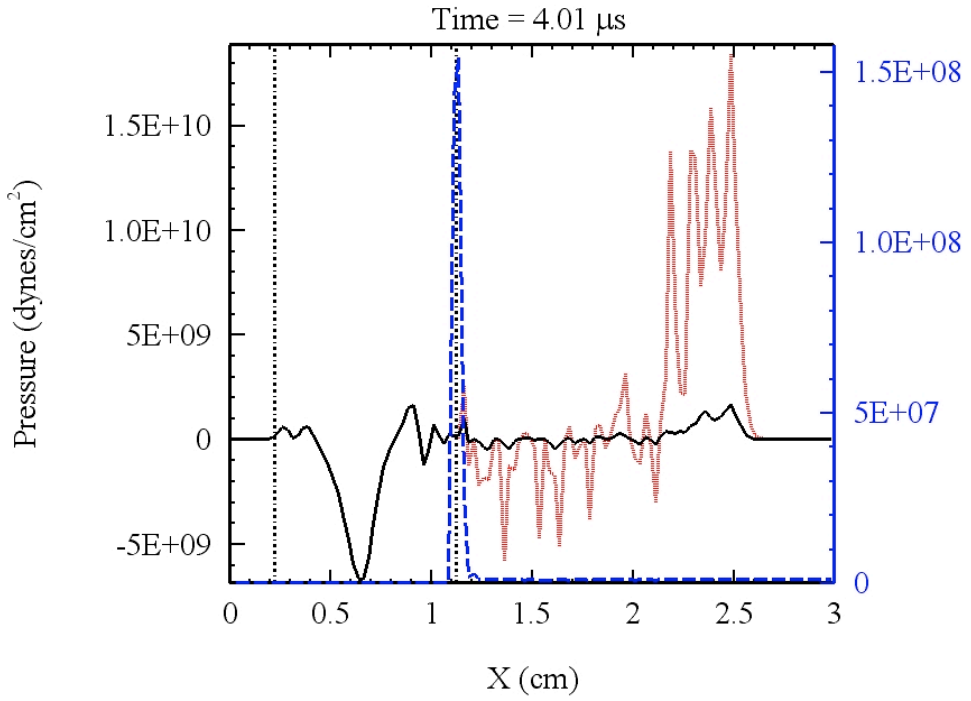

Figure 2. Computational results showing unstable wave propagation into the two-material region.

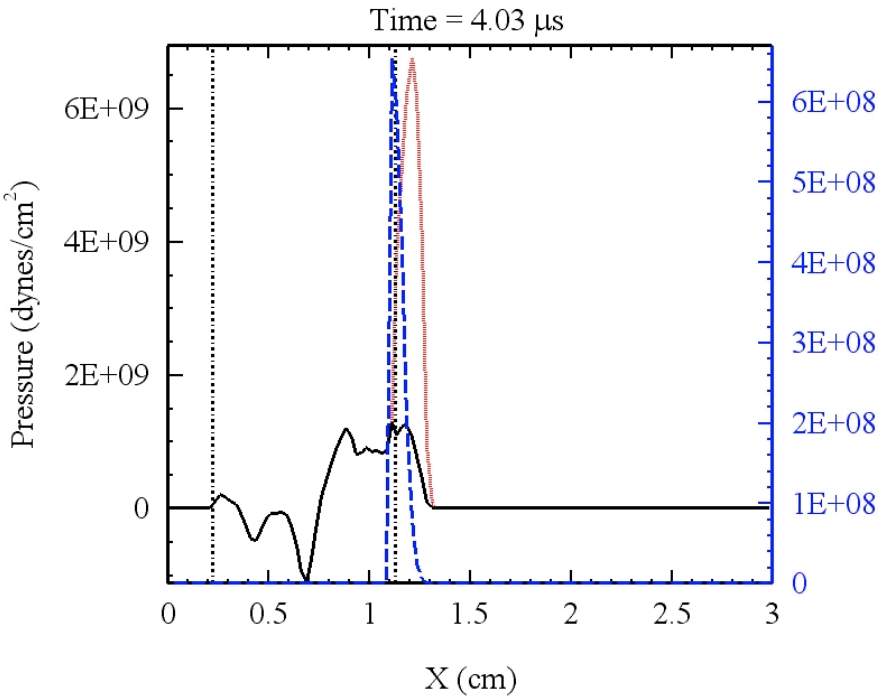

Figure 3. Computational results with the volume fraction evolutionary equation showing stable wave propagation into the two-material region.

➢ Multidimensional problems offer greater potential for generating incorrect numerical results in multimaterial cells. The reasons for this are associated with an increased number of mixed computational cells, more complex motions, and more difficult to quantify stability limits of the underlying numerical methods. However, with more complex motions additional numerical approximations can promote changes or "healing" in energy density states that reduce numerical difficulties. When numerical issues do not "heal" they usually proliferate. Various hydrocodes contain algorithms and methods to reduce the influence of bad thermodynamic cells on the overall computational results. When the number of computational cells with problems grows too large or the numerical results cause the time step to drop then the calculations cannot proceed without action. Sometimes it is possible to adjust the control parameters like the time step or fracture settings. Often the problematic material is discarded, but it is necessary to carefully assess the role of this violation of fundamental laws on the computational results.

➢ The simple two-dimensional problem illustrated in Figure 4 is used to assess the role of the volume fraction evolutionary equation. This problem is a two-dimensional rectangular geometry with four rods moving toward the center of a cylinder of fluid. The rods are a high density solid (platinum) and the fluid is water. Without the volume fraction equation this problem creates nearly two thousand thermodynamic states that generate error conditions. The computational results shown in Figure 5 represent a material plot with the cells that have errors shaded. Notice that for this simulation the symmetry of the solution is broken by the error states. The computational results with the

volume fraction evolutionary equation are presented in Figure 6. The number of thermodynamic states leading to errors is reduced to twelve. All twelve error conditions were the result of a single material cell expansion into tensile states beyond the equation of state applicability. In addition, the computational results maintain similarity and appear to be more consistent.

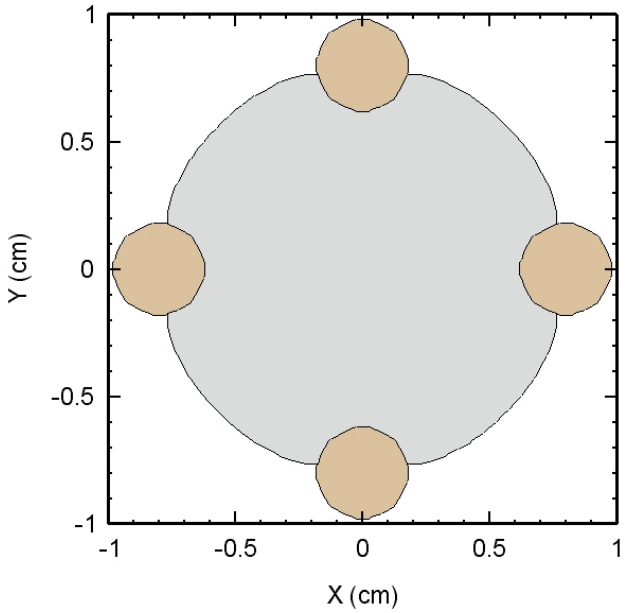

Figure 4. Initial conditions are shown for the two-dimensional rectangular problem with four rods moving toward the center of a cylinder of water.

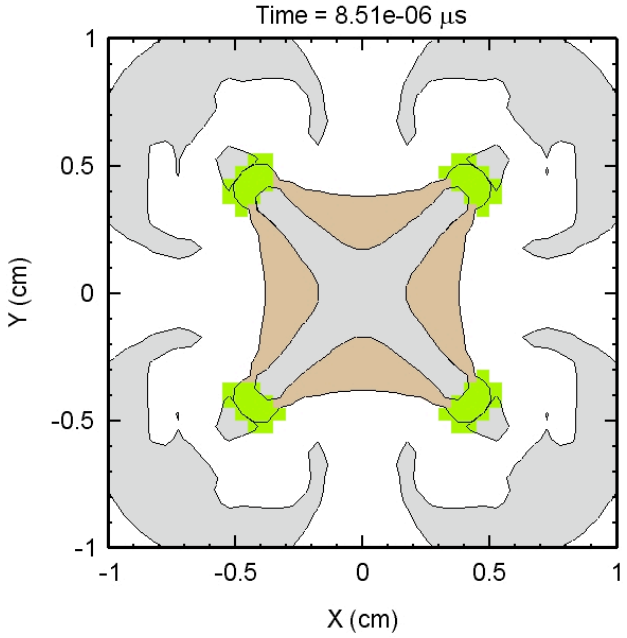

Figure 5. Computational results without the volume fraction evolutionary equation showing computational cells with bad thermodynamic states and broken symmetry.

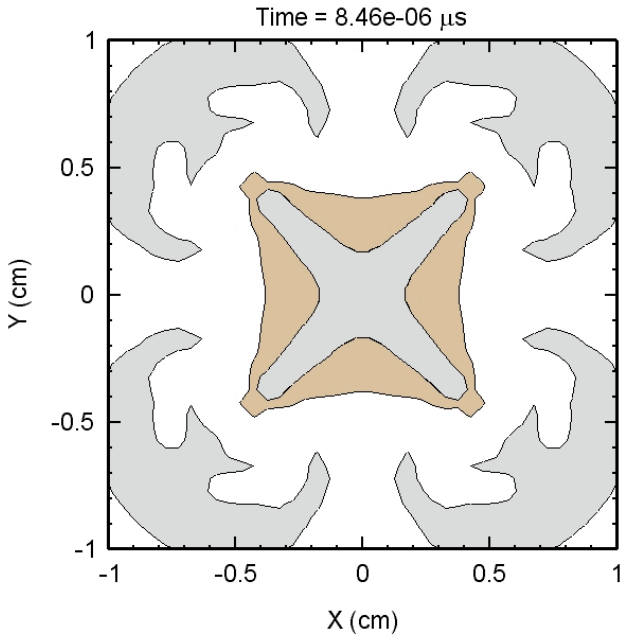

Figure 6. Computational results with the volume fraction evolutionary equation showing better symmetry.

Summary and Conclusions

The addition of an evolutionary equation for the volume fraction was demonstrated to reduce the number of equation of state errors and stabilize an extreme example of a one-dimensional shock propagation problem through a region of space occupied by two materials. The additional equations also offer the opportunity to add in approximations to the "missing" physics represented by intermaterial pressure relaxation and heat transfer. Future efforts will also investigate the possibility of using this paradigm for simulating the processes associated with chemical transformation, phase transformation, porosity evolution, configurational effects, and fracture mechanics. Work that quantifies the statistical processes associated with wave propagation through heterogeneous media demonstrates the need for multimaterial velocity fields and configurational effects. These processes will drive the future development of the volume fraction evolutionary equation addition to traditional shock physics analysis codes.

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References

Andrianov, N., "Analytical and Numerical Investigation of two-phase flows," Dissertation, Otto-von-Guericke Universitat Magdeurg, (2003).

Baer, M. R. and Nunziato, J.W., "A Two-Phase Mixture Theory for the Deflagration-to-Detonation Transition (DDT) in Reactive Granular Materials," Int. J. Multiphase Flow, Vol. 12, no. 6, pp. 861-889, (1986).

Baer, M. R. and Gross, R. J., "A Two-Dimensional Flux-Corrected Transport Solver for Convectively Dominated Flows," Sandia National Laboratories Report, SAND85-0613 UC-32, (1989).

Baer, M.R., "Theoretical and Experimental Studies of the Mesoscale Response of Shock-Loaded Explosive Materials", presented at the 3rd Joint Meeting of the U.S. Section of the Combustion Institute, (2003).

Baty, R. S., "Nonlinear Generalized Functions and Nonconservative Shock Simulations," Sandia National Laboratories Report, SAND94-2258 UC-705, (1994).

Crawford, D.A. and Hensinger, D.M., "Overview of Eulerian Methods and Block Adaptive Mesh Refinement Techniques at Sandia," Proceedings of the Five-Laboratory Conference on Computational Mathematics, Vienna, Austria, 19– 23 June 2005 (2005).

Fromm, J. E., "Lagrangian Difference Approximations for Fluid Dynamics," Los Alamos Scientific Laboratory Report, LA-2535, (1961).

McGlaun, J. M., F. J. Zeigler and S. L. Thompson, "CTH: A Three-Dimensional, Large Deformation, Shock Wave Physics Code", APS Topical Conference on Shock Waves in Condensed Matter, Monterey, CA, July 20-23, (1987).

Miller, G. H. and Colella, P., "A High-Order Eulerian Godunov Method for Elastic-Plastic Flow in Solids," Journal of Computational Physics, vol. 167, pp.131-176, (2001).

Miller, G. H. and Colella, P., "A Conservative Three-Dimensional Eulerian Method for Coupled Solid-Fluid Shock Capturing," Journal of Computational Physics, vol. 183, pp.26-82, (2002).

Miller, G. H. and Puckett, E. G., "A High-Order Godunov Method for Multiple Condensed Phases," Journal of Computational Physics, vol. 128, pp. 134-164, (1996).

Mott, D. R. and Oran. E. S., "CHEMEQ2: a Solver for the Stiff Ordinary Differential Equations of Chemical Kinetics," Naval Research Laboratory Report, NRL/MR/6400—01-8553, (2001).

Oran, E.S. and Boris, J.P., *Numerical Simulation of Reactive Flow*, Elsevier, New York, (1987).

Saurel, R. and Abgrall, R. "A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows," Journal of Computational Physics, vol. 150, pp. 425-467, (1999).

Shampine, L.F. and Watts, H.A., "DEPAC-Design of a User Oriented Package for ODE Solvers," Sandia National Laboratories Report, SAND79-2374, Sandia National Laboratories, Albuquerque, New Mexico, (1980).

Shuvalov, V. V., Artem'eva, N. A., Kosarev, I. B., "3D Hydrodynamic Code SOVA for Multimaterial Flows, Applications to Shoemaker-Levy 9 Comet Impact Problem," International Journal of Impact Engineering, vol. 23, pp. 847-858, (1999).

Stone, J.M. and Norman, M.I., "ZEUS-2D: A Radiation Magnetohydrodynamics Code For Astrophysical Flows in Two Space Dimensions. I. The Hydrodynamic Algorithms and Tests," The Astrophysical Journal Supplement Series, Vol. 80: pp. 53-790, (1992).

Truesdell, C., *Rational Thermodynamics*, McGraw-Hill, New York, (1984).

Van Leer, B., "Towards the Ultimate Conservative Difference scheme IV. A New Approach to Numerical Convection," Journal of Computational Physics, vol. 23, pp. 276-299, (1977).

Van Leer, B., "Towards the Ultimate Conservative Difference scheme V. A Second-Order Sequel to Godunov's Method," Journal of Computational Physics, vol. 32, pp. 101-136, (1979).

Yee, H. C. "Construction of Explicit and Implicit Symmetric TVD Schemes and Their Application," Journal of Computational Physics, Vol. 68, pp. 151-179, (1987).

Yanenko, N.N., *The Method of Fractional Steps*, Springer-Verlag, New York, (1971).